On shielding of nuclear electric dipole moments in atoms

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Abstract

We demonstrate explicitly that some recent calculations of atomic electric dipole moments (EDM) are incomplete. A contribution overlooked therein is pointed out. When included, it cancels exactly the result of those calculations, and thus restores the standard conclusions for nuclear EDM in atoms.

The existence of EDMs of elementary particles, nuclei, and atoms is forbidden by CP invariance. The predictions of the standard model of electroweak interactions for these EDMs are at least six orders of magnitude below the present experimental bounds. It makes experimental searches for EDMs, even at present level of accuracy, extremely sensitive to possible new physics beyond the standard model.

The best upper limit on EDM of anything was obtained on the ^{199}Hg atomic dipole moment [1]:

$$d(^{199}\mathrm{Hg}) < 2.1 \times 10^{-28}\ e\ \mathrm{cm}. \tag{1}$$

Unfortunately, the implications of this result for the dipole moment of the valence neutron of the ^{199}Hg nucleus is much less impressive [2]:

$$|d_n| < 4.0 \times 10^{-25}\ e\ \mathrm{cm} \tag{2}$$

(still, it is not so far away from the results of the direct measurements of the neutron EDM [3, 4]: $|d_n| < (0.6 - 1.0) \times 10^{-25}\ e$ cm).

The explanation is as follows. For a neutral atom of point particles, in equilibrium under the action of electrostatic forces, there is no effect due to the EDMs of the constituent particles [5, 6]. Indeed, the atom remains at rest when an external electric field $\mathbf{E}_{ext}$ is applied. This comes about by an internal rearrangement of the system's constituents giving rise to an internal field $\mathbf{E}_{int}$ that exactly cancels $\mathbf{E}_{ext}$ at each charged particle, as required by the static equilibrium condition. Thus, there is no observable effect due to dipole moments of the system's constituents; the external field is effectively switched off.

A quantum mechanical proof of this statement was given in [7]. It was also pointed out therein that the shielding of atomic nucleus is not complete, observable nuclear EDM effects arise when one takes into account its finite size. Of course, the resulting suppression of these effects is quite

essential. The suppression factor η is roughly the ratio squared of the nuclear radius to that of the atomic K-shell (see, for instance, [8]):

$$\eta \sim \left(\frac{A^{1/3} r_0}{a/Z}\right)^2 \tag{3}$$

(here $a = 0.5 \times 10^{-8}$ cm, $r_0 = 1.2 \times 10^{-13}$ cm). Numerically for the mercury atom $\eta \sim 10^{-4}$, and this is the reason why the strict atomic upper limit (1) reduces to much milder neutron one (2).

However, this conclusion was revised in recent papers [9, 10]. The relations between atomic and neutron EDMs advocated therein are as follows:

$$d(^{199}\mathrm{Hg}) \simeq -2.8 d_n, \tag{4}$$

$$d(^{129}\mathrm{Xe}) \simeq 1.6 d_n, \tag{5}$$

$$d(\mathrm{D}) \simeq 0.017 d_n, \tag{6}$$

where $d(^{129}\mathrm{Xe})$, $d(^{199}\mathrm{Hg})$, and $d(\mathrm{D})$ are the EDMs of xenon, mercury, and deuterium atoms, respectively. In particular, from the upper limit (1) for the dipole moment of mercury atom the authors of [9] extract a very strict bound on the neutron EDM

$$d_n \simeq (0.37 \pm 0.17 \pm 0.14) \times 10^{-28}\, e \text{ cm}. \tag{7}$$

If results (4) – (7) were correct, they would be, as discussed at length in [10], of paramount importance for the problem of CP violation (as well as for the present programs of searches for the neutron, nuclear and atomic EDMs). This is why we believe that it is proper to analyze attentively the arguments of [9]. To make our discussion as simple and transparent as possible, we confine it to the case of deuterium (where relation (6) differs from that following from estimate (3) by 8 orders of magnitude). An important contribution to the atomic EDM overlooked in [9] is pointed out, which exactly cancels the contribution considered therein. So, let us discuss in detail how the shielding works.

The unperturbed deuterium Hamiltonian is

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{|\mathbf{r} - \mathbf{R}/2|} + \frac{\mathbf{P}^2}{M} + U(\mathbf{R}, \mathbf{S}). \tag{8}$$

Here $\mathbf{p}$ and $\mathbf{r}$ are the momentum and coordinate of electron, $\mathbf{P}$ and $\mathbf{R}$ are the relative momentum and coordinate of the nucleons, $U(\mathbf{R}, \mathbf{S})$ is the strong proton-neutron potential (by the way, it depends essentially on the total spin $\mathbf{S}$ of the nucleons); all coordinates are counted off the center of mass of the deuteron. We confine here and below to the nonrelativistic limit, which is quite sufficient for our purpose.

To separate the atomic and nuclear variables, we rewrite Hamiltonian (8) as $H = H_a + H_N + W$, where

$$H_a = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r} \tag{9}$$

is the atomic Hamiltonian,

$$H_N = \frac{\mathbf{P}^2}{M} + U(\mathbf{R}, \mathbf{S}). \tag{10}$$

is the nuclear one; perturbation

$$W = -\frac{e^2}{|\mathbf{r} - \mathbf{R}/2|} + \frac{e^2}{r} = \frac{\mathbf{R}}{2} \boldsymbol{\nabla} \frac{e^2}{r} = -\frac{\mathbf{R}}{2}\, i\, [\mathbf{p}, H_a] \tag{11}$$

is treated to first order in R/r only.

The next perturbation describes the interaction of the electron and proton charges with an external electric field $\mathbf{E}_{ext}$:

$$V = e\left(\mathbf{r} - \frac{\mathbf{R}}{2}\right)\mathbf{E}_{ext}\,; \tag{12}$$

here and below $e = e_p > 0$.

And at last, we present the P odd and T odd interaction of the neutron EDM $\mathbf{d}_n$ with the Coulomb field of the proton considered in [9]:

$$v = e\,\frac{\mathbf{d}_n\mathbf{R}}{R^3}\,. \tag{13}$$

When combined with perturbation (12), it results in the following second-order contribution to the deuteron EDM:

$$\mathbf{d}_2 = \sum_n \frac{\langle 0|e\mathbf{R}/2|n\rangle\langle n|v|0\rangle}{E_0 - E_n} + \text{h.c.}\,. \tag{14}$$

Of course, only that part of perturbation (12)

$$V_1 = -e\,\frac{\mathbf{R}}{2}\,\mathbf{E}_{ext}\,, \tag{15}$$

which depends on the nuclear coordinate $\mathbf{R}$, is operative here. Expression (14) for the nuclear EDM, induced by interaction (13), is certainly correct. Moreover, it is valid for any P odd and T odd proton–neutron interaction, not only for that described by formula (13). In particular, the deuteron EDM induced in this way by the P odd and T odd pion exchange, was calculated in [11].

However, this is the EDM of the nucleus, deuteron, but not the total EDM of the atom, deuterium, which should vanish in the point limit due to the atomic shielding effect pointed out above.

To restore this shielding, we switch on, in line with (12) and (13), perturbation (11). Its matrix element between two atomic states with energies $\varepsilon_2,\ \varepsilon_1$ can be conveniently rewritten as follows:

$$\langle\varepsilon_2|\,W\,|\varepsilon_1\rangle = \frac{i}{2}\,\mathbf{R}\langle\varepsilon_2|\,\mathbf{p}\,|\varepsilon_1\rangle(\varepsilon_2 - \varepsilon_1). \tag{16}$$

As to interaction (12), it obviously reduces in this case to

$$V_2 = e\,\mathbf{r}\mathbf{E}_{ext}. \tag{17}$$

Now we calculate the combined result of interactions (13), (16), and (17). After some rearrangement of terms, using extensively the completeness relation for atomic states, we obtain the following result for this third-order contribution:

$$\mathbf{d}_3 = -\sum_n \frac{\langle 0|e\mathbf{R}/2|n\rangle\langle n|v|0\rangle}{E_0 - E_n} + \text{h.c.}\,. \tag{18}$$

The contributions (14) and (18) cancel, in complete accordance with the shielding theorem. Obviously, the cancellation occurs for any P odd and T odd proton-neutron interaction v.

One should not be surprised by the cancellation between second-order effect (14) and third-order one (18). While perturbation (13) is common for both effects, it can be easily checked that the combined action of perturbations (16) and (17) can well be on the same order of magnitude as that of (15).

In fact, the neutron and proton electric dipole moments, $\mathbf{d}_n$ and $\mathbf{d}_p$, induce the EDM of the atom due to the so-called Schiff moment (SM) [2, 12–14] (SM vanishes, of course, in the limit of point nucleus). The general expression for SM operator, induced by $\mathbf{d}_n$ and $\mathbf{d}_p$, reduces for the deuteron to the following form:

$$S_i = \frac{1}{24}\,(d_{n\,i} + d_{p\,i})\,(R^2 - \langle R^2 \rangle) + \frac{1}{60}\,(d_{n\,j} + d_{p\,j})\,[\,(3R_iR_j - \delta_{ij}R^2) - 4Q_{ij}\,]\,; \tag{19}$$

here $\langle R^2 \rangle$ and Q_{ij} are the expectation values of R^2 and the deuteron quadrupole moment, respectively.

In conclusion, the following peculiarity of the deuteron is worth mentioning. If the strong proton-neutron potential $U(\mathbf{R}, \mathbf{S})$ were independent of the total spin $\mathbf{S}$, we would have, obviously,

$$\langle (d_{n\,i} + d_{p\,i})\,R^2\,\rangle = \langle\, d_{n\,i} + d_{p\,i}\,\rangle\,\langle R^2 \rangle, \quad \text{and} \quad \langle (d_{n\,j} + d_{p\,j})\,(3R_iR_j - \delta_{ij}R^2)\,\rangle = 4\langle\, d_{n\,j} + d_{p\,j}\,\rangle\,Q_{ij}\ .$$

Therefore, in this case the expectation value of the deuteron Schiff moment (19), generated by $\mathbf{d}_n$ and $\mathbf{d}_p$, would vanish, and together with it the atomic deuterium EDM would vanish as well.

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